(FILE 'HOME' ENTERED AT 16:11:03 ON 09 AUG 2007)

FILE 'REGISTRY' ENTERED AT 16:14:38 ON 09 AUG 2007

L1 STRUCTURE UPLOADED

L2 4 S L1 SSS SAM

L3 68 S L1 SSS FULL

FILE 'HCAPLUS' ENTERED AT 16:15:17 ON 09 AUG 2007

L4 21 S L3

L5 415133 S VIRUS OR ANTIVIRAL OR HIV

L6 4 S L4 AND L5 E SPERM+ALL/CT

·

=> s 14 not 16

L7 17 L4 NOT L6

=> s sperm?

L8 77500 SPERM? .

=> s 18 an d14

MISSING OPERATOR L8 AN

The search profile that was entered contains terms or nested terms that are not separated by a logical operator.

=> s 18 and 14

L9 4 L8 AND L4

=> s 19 not 16

L10 0 L9 NOT L6

=> s vag?

L11 43957 VAG?

=> s 111 and 14

L12 2 L11 AND L4

=> s 112 not 16

L13 0 L12 NOT L6

=> d 17 ibib abs hitstr 1-17

=> d l7 ibib abs hitstr 1-17

```
L7
     ANSWER 1 OF 17 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:
                            2007:703781 HCAPLUS <<LOGINID::20070809>>
DOCUMENT NUMBER:
                            147:116578
TITLE:
                            Sophorolipids as protein inducers and inhibitors in
                            fermentation medium
INVENTOR (S):
                            Gross, Richard A.; Shah, Vishal; Nerud, Frantisek;
                            Madamwars, Datta
PATENT ASSIGNEE(S):
                            Polytechnic University, USA
SOURCE:
                            PCT Int. Appl., 12pp.
                            CODEN: PIXXD2
DOCUMENT TYPE:
                            Patent
LANGUAGE:
                            English
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
      PATENT NO.
                            KIND
                                    DATE
                                                  APPLICATION NO.
                                                                            DATE
                            _ _ _ _
                                                  ------
                                                                             ____
      WO 2007073371
                             A1
                                    20070628
                                                  WO 2005-US46457
                                                                            20051222
          W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
               CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
               GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP., KR,
              KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC,
          VN, YU, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
               CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
               KG, KZ, MD, RU, TJ, TM
PRIORITY APPLN. INFO.:
                                                  WO 2005-US46457
                                                                            20051222
     A method for producing sophorolipids having protein inducer and/or
     repressor activities having the steps of synthesizing the sophorolipid by
      fermentation of Candida bombicola in a fermentation media to form a natural mixture of
      lactonic sophorolipids and non-lactonic sophorolipids and then utilizing
      the natural mixture as a protein inducing agent, utilizing the natural mixture
      as a protein repressing agent, and/or utilizing the natural mixture as a
      combined protein induction/repressor agent. An application of the
      sophorolipid compound produced according to the method as a microbial media
      component.
IT
      805250-88-8P 805250-89-9P 942630-33-3P
      942630-34-4P
     RL: BPN (Biosynthetic preparation); BUU (Biological use, unclassified);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
         (sophorolipids as protein inducers and inhibitors in fermentation medium)
      805250-88-8 HCAPLUS
RN
CN
      9-Octadecenoic acid, 17-[(2-O-β-D-glucopyranosyl-β-D-
     glucopyranosyl)oxy] - (CA INDEX NAME)
```

HO
$$_{\rm R}$$
 $_{\rm R}$ $_{\rm CH_2}$ $_{\rm OH}$ $_{\rm OH}$ $_{\rm CH_2}$ $_{\rm OH}$ $_{\rm OH}$ $_{\rm OH}$ $_{\rm OH}$ $_{\rm OH}$

RN 805250-89-9 HCAPLUS

CN 9-Octadecenoic acid, 17-[[6-O-acetyl-2-O-(6-O-acetyl- β -D-glucopyranosyl)- β -D-glucopyranosyl] oxy] - (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

RN 942630-33-3 HCAPLUS CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

Double bond geometry unknown.

RN 942630-34-4 HCAPLUS CN INDEX NAME NOT YET ASSIGNED Absolute stereochemistry.

Double bond geometry unknown.

HO
$$_{\rm C}$$
 $_{\rm CH_2}$ $_{\rm C}$ $_{\rm CH_2}$ $_{\rm CH_2}$ $_{\rm C}$ $_{\rm CH_2}$ $_{\rm CH_2}$ $_{\rm C}$ $_{\rm CH_2}$ $_{\rm$

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 17 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:1143610 HCAPLUS <<LOGINID::20070809>>

DOCUMENT NUMBER: 144:291342

TITLE: Sophorolipid biosynthesis from a biodiesel co-product

stream

AUTHOR(S): Ashby, Richard D.; Nunez, Alberto; Solaiman, Daniel K.

Y.; Foglia, Thomas A.

CORPORATE SOURCE: Fats, Oils and Animal Coproducts Research Unit, ARS,

ERRC, USDA, Wyndmoor, PA, 19038, USA

SOURCE: Journal of the American Oil Chemists' Society (2005),

82(9), 625-630

CODEN: JAOCA7; ISSN: 0003-021X

PUBLISHER: AOCS Press
DOCUMENT TYPE: Journal
LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:291342

We applied a biodiesel co-product stream (BCS) as a fermentation feedstock for the microbial synthesis of sophorolipids (SL). The BCS was composed of 40% glycerol, 34% hexane-solubles (made up of 92% FA soaps/FAME and 6% MAG/DAG), and 26% water. Batch culture fermns. of the yeast Candida bombicola on pure glycerol resulted in low-level synthesis of SL (.apprx.9 g/L). HPLC associated with atmospheric pressure CI-MS (LC/APCI-MS) revealed that the SL derived from pure glycerol had 99% of the FA side chains linked to the 4'' hydroxyl group of the sophorose sugar, resulting in a lactonic structure. In contrast, the use of the BCS as feedstock increased the SL yield to 60 g/L and the open-chain form to 75% including both oleic acid and linoleic acid (along with their Me esters) as the dominant species comprising the side chains. By favoring the open-chain structure, the SL mols. (particularly the FA side chain) can be chemical modified without the need to open a lactone ring first. The ability to use the BCS as a feedstock for SL synthesis will provide an outlet for this residual material, thus helping to stimulate growth in the biodiesel market and the use of agricultural fats and oils from which the biodiesel was synthesized.

IT 821800-26-4P 879012-92-7P

RL: BMF (Bioindustrial manufacture); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)

(sophorolipid biosynthesis from biodiesel co-product stream)

RN 821800-26-4 HCAPLUS

CN 9-Octadecenoic acid, 17-[[6-O-acetyl-2-O-(6-O-acetyl- β -D-

glucopyranosyl)- β -D-glucopyranosyl]oxy]-, methyl ester, (9Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

ACO OH OH OH OH

$$R$$
 S R OH R S R OH OH

 R S R OH OH

 R OH OH

 R OH OH

RN 879012-92-7 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-, methyl ester, (9Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

MeO (CH₂) 7
$$\underline{Z}$$
 (CH₂) 6 O OH OH

REFERENCE COUNT:

THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 17 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

DOCUMENT NUMBER:

142:43453

TITLE:

Cosmetic uses of sophorolipids as agents for

regulating subcutaneous adipose mass and slimming

INVENTOR (S):

Pellicier, Francoise; Andre, Patrice

PATENT ASSIGNEE(S):

Lvmh Recherche, Fr. Fr. Demande, 32 pp.

SOURCE: Fr. Demande, 3
CODEN: FRXXBL

DOCUMENT TYPE:

Patent

LANGUAGE:

French

FAMILY ACC. NUM. COUNT:

1

PATENT INFORMATION:

PATENT NO.

KIND DATE

APPLICATION NO.

DATE

```
FR 2855752
                       A1
                              20041210
                                           FR 2003-6664
                                                                     20030603
FR 2855752
                       B1
                              20050826
WO 2004108063
                                           WO 2004-FR1359
                                                                     20040602
                       A2
                              20041216
WO 2004108063
                       A3
                              20050127
        AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
         CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
         GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
         LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
         NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
         TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
    RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
        AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
         SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
         SN, TD, TG
```

PRIORITY APPLN. INFO.:

FR 2003-6664 A 20030603

OTHER SOURCE(S): MARPAT 142:43453

New cosmetic uses of the sophorolipids, as slimming agents stimulating the synthesis of the leptin by the adipocytes are disclosed. The cosmetic compns. contain at least 1 sophorolipid and a lipolytic agent selected from the compds., c-AMP and its derivs. Thus, an emulsion contained polypropylene glycol isoceteth-20 acetate 2, Poloxamer-407 0.50, propylene glycol isoceteth-3 acetate 15, pentacyclomethicone 15, butylene glycol 3, preservative qs, Coleus forskohlii extract 0.1, xanthan gum 0.05, acrylate-C10-30/alkyl acrylate copolymer 0.04, polyacrlamide C13-14 isoparaffin laureth-7 0.50, perfume 0.20, Sopholiance 0.50 and water qs to 100%.

IT 805250-88-8 805250-89-9

> RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses) (cosmetic use of sophorolipids as agents for regulating s.c. adipose mass and slimming).

RN805250-88-8 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-O-β-D-glucopyranosyl-β-Dglucopyranosyl)oxy] - (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

RN805250-89-9 HCAPLUS

CN 9-Octadecenoic acid, 17-[[6-O-acetyl-2-O-(6-O-acetyl-β-Dglucopyranosyl)- β -D-glucopyranosyl]oxy]-. (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 17 HCAPLUS COPYRIGHT 2007 ACS on STN

3

ACCESSION NUMBER:

2004:905607 HCAPLUS <<LOGINID::20070809>>

DOCUMENT NUMBER:

141:355428

TITLE:

Treatment and prophylaxis of sepsis and septic shock

with sophorolipids

INVENTOR(S):

Gross, Richard A.

PATENT ASSIGNEE(S):

USA

SOURCE:

U.S. Pat. Appl. Publ., 10 pp.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PA	PATENT NO.						DATE		APPLICATION NO.					DATE					
. 110	US 2004214795					_				110 2004 007061									
							20041028		00 2001 007501										
					A1		20051013			CA 2005-2557671				20050324					
					A2 200510:									20050324					
WO	O 2005094268				A3	A3 20070426													
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,		
							DE,												
							ID,												
							LV,												
							PL,												
		SY,	Τυ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW,	US	
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	ŪĠ,	ZM,	ZW,	AM,		
		ΑZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,		
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,	IS,	IT,	LT,	LU,	MC.	NL.	PL.	PT.		
							BF,												
											/	J,	J,	U11 ,	OQ,	· ,	,		
ED						TD, TG, AP, EA,			EP 2005-730352					20050224					
111	D. AM DE DA			A2 20061213			DK, EE, ES, FI, FR,				20050324								
	K:	A1,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,		
						LU,	MC,	ΝL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	AL,	BA,		
		HR,	LV,	MK,	YU														
PRIORIT				US 2003-457070P					P 20030324										
										US 2004-807961									
	WO 2005-US10060																		
			_	_			_		. '	Z	000-		000	W 20050324					

AB A composition for the prophylaxis or treatment of humans or animals for septic shock and sepsis using a mixture of sophorolipids is disclosed. The in vivo expts. demonstrated that sophorolipids have a protective effect against ongoing endotoxic shock. I.p. injection of sophorolipids 1.5 h after galactosamine-LPS treatment resulted in 53% lower mortality than that observed among pos. control mice.

IT 220608-02-6 220608-11-7 693786-10-6

777091-27-7

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (treatment and prophylaxis of sepsis and septic shock)

RN 220608-02-6 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-0- β -D-glucopyranosyl- β -D-

glucopyranosyl)oxy]-, ethyl ester, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 220608-11-7 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-0- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

HO
$$_{\rm R}$$
 $_{\rm R}$ $_{\rm R}$ $_{\rm OH}$ $_{\rm OH}$

RN 693786-10-6 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-, hexyl ester, (9Z,17S)- (9CI) (CA INDEX NAME)

Me (CH₂)
$$\frac{OH}{5}$$
 (CH₂) $\frac{CH_2}{5}$ (CH₂)

RN 777091-27-7 HCAPLUS

CN 9-Octadecenoic acid, 17-[[6-O-acetyl-2-O-(6-O-acetyl- β -D-glucopyranosyl)- β -D-glucopyranosyl]-, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

L7 ANSWER 5 OF 17 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:603194 HCAPLUS <<LOGINID::20070809>>

DOCUMENT NUMBER: 141:290899

TITLE: Supramolecular Assemblies of a Naturally Derived

Sophorolipid

AUTHOR(S): Zhou, Shuiqin; Xu, Chang; Wang, Jun; Gao, Wei;

Akhverdiyeva, Rena; Shah, Vishal; Gross, Richard

CORPORATE SOURCE: Department of Chemistry, Institute of Macromolecular

Assembly, College of Staten Island, City University of

New York, Staten Island, NY, 10314, USA

SOURCE: Langmuir (2004), 20(19), 7926-7932

CODEN: LANGD5; ISSN: 0743-7463

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Acidic sophorolipid (SL) mols. derived from yeasts represent a novel type of asym. bolaamphiphiles due to their unique structural features that include an asym. polar head size (disaccharide vs COOH), a kinked hydrophobic core (cis-9-octadecenoic chain), and a non-amide polar-nonpolar linkage. Light microscopy, small- and wide-angle X-ray scattering, FT-IR spectroscopy, and dynamic laser light scattering were used to investigate the supramol. structures of the self-assembled

aggregates of SL mols. at different pH values. In acidic conditions (pH < 5.5), giant twisted and helical ribbons of 5-11 μm width and several hundreds of micrometers length were observed for the first time. Increase in solution pH values slowed ribbon formation, decreased ribbon yield, and increased the helicity and entanglements of the giant ribbons. An interdigitated lamellar packing model of acidic SL-COOH mols. with a long period of 2.78 nm, stabilized by both the strong hydrophobic association between the cis-9-octadecenoic chains and strong disaccharide-disaccharide hydrogen bonding, is proposed. The neutralization of SL-COOH in water to SL-COONa produced clear solns. with the formation of short-range ordered aggregates. At concns. below 1.0 mg/mL, the size of self-assembled aggregates increased as the concentration increased. At concns. above 1.0 mg/mL, narrowly distributed micellar aggregates with a constant hydrodynamic radius (Rh) of about 100 nm are formed. The large micelles show strong angular dependence with the fast mode appearing at scattering angle θ ≥ 60°.

IT 220608-11-7

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(supramol. assemblies of naturally derived acidic sophorolipid from Candida bombicola)

RN 220608-11-7 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 6 OF 17 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:500268 HCAPLUS <<LOGINID::20070809>>

DOCUMENT NUMBER: 142:112516

TITLE: Synthesis and interfacial properties of sophorolipid

derivatives

AUTHOR(S): Zhang, Lei; Somasundaran, P.; Singh, Sanjay K.; Felse,

Arthur P.; Gross, Richard

CORPORATE SOURCE: NSF Industry/University Cooperative Research Center

for Advanced Studies on Novel Surfactant, School of Engineering and Applied Sciences, Columbia University,

New York, NY, 10027, USA

SOURCE: Colloids and Surfaces, A: Physicochemical and

Engineering Aspects (2004), 240(1-3), 75-82

CODEN: CPEAEH; ISSN: 0927-7757

PUBLISHER: Elsevier DOCUMENT TYPE: Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 142:112516

Biosurfactants made by fermentation from renewable resources provide "environmentally friendly" processes and products. A natural sophorolipid mixture was produced by the yeast Candida bombicola when cultured on glucose and oleic acid. The sophorolipid mixture was chemical modified to form the corresponding sophorolipid alkyl (Me, Et, Pr, and butyl) esters by reaction with the corresponding sodium alkoxides. Interfacial properties of these surfactants, such as surface tension reduction, aggregation, and adsorption, were systematically studied. It was found that the critical micelle concentration of sophorolipid esters decreases to about 1/2 per addnl. one CH2 group to the alkyl ester moiety. Interestingly, these surfactants were found to adsorb strongly on alumina but weakly on silica. They have properties that make them attractive candidates for uses in detergents, cosmetics, soil remediation, and enhanced oil recovery.

IT 821800-26-4P 821800-40-2P 821800-54-8P

821800-55-9P 821800-56-0P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (synthesis and interfacial properties of sophorolipid derivs.)

RN821800-26-4 HCAPLUS

CN9-Octadecenoic acid, 17-[[6-O-acetyl-2-O-(6-O-acetyl-β-Dglucopyranosyl)-β-D-glucopyranosyl]oxy]-, methyl ester, (9Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 821800-40-2 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-O-β-D-glucopyranosyl-β-Dglucopyranosyl)oxy]-, ethyl ester, (9Z)- (9CI) (CA INDEX NAME)

RN 821800-54-8 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-, propyl ester, (9Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

$$n$$
-PrO (CH₂) 7 Z (CH₂) 6 O OH

RN 821800-55-9 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-, butyl ester, (9Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 821800-56-0 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-0- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-, hexyl ester, (9Z)- (9CI) (CA INDEX NAME)

Me (CH₂)
$$\frac{OH}{5}$$
 (CH₂) $\frac{OH}{5}$ (CH₂)

REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 7 OF 17 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:729051 HCAPLUS <<LOGINID::20070809>>

DOCUMENT NUMBER: 140:2333

TITLE: Enzyme-catalyzed regioselective transesterification of

peracylated sophorolipids

AUTHOR(S): Carr, Jason A.; Bisht, Kirpal S.

CORPORATE SOURCE: Department of Chemistry, University of South Florida,

Tampa, FL, 33620, USA

SOURCE: Tetrahedron (2003), 59(39), 7713-7724

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:2333

Regioselective transesterifications and hydrolysis of peracylated sophorolipid (SL) derivs. catalyzed by lipases was investigated. This study is the first evaluation of the lipase-catalyzed reactions on the non-lactonic SL derivs. Four lipases, namely from porcine pancreas (PPL, Type II), Candida rugosa (AYS, TypeVII), Pseudomonas cepacia (PS-30), and Candida antarctica (Novozym 435, carrier fixed lipase fraction B) were used in anhydrous THF or in phosphate buffer (pH=7.4, 0.2 M). It was confirmed from the detailed spectral anal. of the products that transesterification failed to furnish any free hydroxyls on the sophorose Instead, transesterification took place on the Me ester located at the carboxylic end of the 17-hydroxyoctadecenoic acid chain attached to the C-1' position of the sophorose ring. It is proposed that in absence of the lactonic structural motif, the binding of the peracylated non-lactonic SLs in the lipase binding pocket takes place such that the carboxyl group of the octadecenoic acid, not the sophorose sugar, is preferentially accessible to the active site.

IT 220608-04-8P

RL: BPN (Biosynthetic preparation); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(lipase-catalyzed regioselective transesterification of peracylated sophorolipids)

RN 220608-04-8 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-, butyl ester, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

IT 213754-46-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PRÉP (Preparation); RACT (Reactant or reagent)

(lipase-catalyzed regioselective transesterification of peracylated sophorolipids)

RN 213754-46-2 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-0- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-, methyl ester, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

MeO (CH₂) 7
$$\underline{Z}$$
 (CH₂) 6 \underline{S} O OH OH

REFERENCE COUNT:

THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 8 OF 17 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:577657 HCAPLUS <<LOGINID::20070809>>

DOCUMENT NUMBER: 140:164079

TITLE:

Enzymatic synthesis of a galactopyranose sophorolipid

fatty acid-ester

AUTHOR(S): Nunez, Alberto; Foglia, Thomas A.; Ashby, Richard CORPORATE SOURCE: Eastern Regional Research Center, US Department of

Agriculture, Fats, Oils and Animal Coproducts Research Unit, Agricultural Research Service, Wyndmoor, PA,

19038, USA

SOURCE: Biotechnology Letters (2003), 25(16), 1291-1297

CODEN: BILED3; ISSN: 0141-5492

PUBLISHER: Kluwer Academic Publishers

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:164079

AB Sophorolipid lactones produced by Candida bombicola were deacetylated and ring opened with sodium methoxide to their corresponding Me esters. The Me esters, after re-acetylation with vinyl acetate using an immobilized lipase, were transesterified with 1,2-3,4-di-O-isopropylidene-dgalactopyranose in THF using the same lipase catalyst. The di-O-isopropylidene sophorolipid sugar esters were hydrolyzed to give the galactopyranose sophorolipid esters as the final products. IT 220608-06-0P 655232-87-4P 655232-90-9P 655232-91-0P 655232-92-1P 655232-94-3P RL: BPN (Biosynthetic preparation); RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent) (enzymic preparation of galactopyranose sophorolipid esters) RN 220608-06-0 HCAPLUS CN 9-Octadecenoic acid, 17-[[6-O-acetyl-2-O-(6-O-acetyl-β-Dglucopyranosyl)-β-D-glucopyranosyl]oxy]-, methyl ester, (92,178)-

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

(9CI) (CA INDEX NAME)

RN 655232-87-4 HCAPLUS CN α -D-Galactopyranose, 1,2:3,4-bis-O-(1-methylethylidene)-, (9Z,17S)-17-[[6-O-acetyl-2-O-(6-O-acetyl- β -D-glucopyranosyl)- β -D-glucopyranosyl]oxy]octadecanoate (9CI) (CA INDEX NAME)

PAGE 1-B

....ОН

RN 655232-90-9 HCAPLUS CN α -D-Galactopyranose, 1,2:3,4-bis-O-(1-methylethylidene)-,

(9Z,17S)-17-[[2-O-(6-O-acetyl-β-D-glucopyranosyl)-β-D-glucopyranosyl]oxy]-9-octadecenoate (9CI) (CA INDEX NAME)

PAGE 1-B

RN 655232-91-0 HCAPLUS

CN α -D-Galactopyranose, 1,2:3,4-bis-O-(1-methylethylidene)-, (9Z,17S)-17-[(6-O-acetyl-2-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-9-octadecenoate (9CI) (CA INDEX NAME)

PAGE 1-B

....ОН

RN 655232-92-1 HCAPLUS

CN α -D-Galactopyranose, 1,2:3,4-bis-O-(1-methylethylidene)-, (9Z,17S)-17-[(2-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-9-octadecenoate (9CI) (CA INDEX NAME)

PAGE 1-B

RN 655232-94-3 HCAPLUS

CN 9-Octadecenoic acid, 17-[(6-O-acetyl-2-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-, methyl ester, (9Z,17S)- (9CI) (CA INDEX NAME)

IT 655232-89-6P

RL: BPN (Biosynthetic preparation); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(enzymic preparation of galactopyranose sophorolipid esters)

RN 655232-89-6 HCAPLUS

CN α -D-Galactopyranose, 6-[(9Z,17S)-17-[(2-O- β -D-glucopyranosyl-

 β -D-glucopyranosyl)oxy]-9-octadecenoate] (9CI) (CA INDEX NAME)

PAGE 1-B

.... OH

∾он

IT 213754-46-2P

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(enzymic preparation of galactopyranose sophorolipid esters)

RN 213754-46-2 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-O- β -D-glucopyranosyl- β -D-

glucopyranosyl)oxy]-, methyl ester, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

MeO (CH₂) 7
$$\underline{Z}$$
 (CH₂) 6 \underline{S} O OH

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 9 OF 17 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:505381 HCAPLUS <<LOGINID::20070809>>

DOCUMENT NUMBER: 139:197675

TITLE: Regioselective Enzyme-Catalyzed Synthesis of

Sophorolipid Esters, Amides, and Multifunctional

Monomers

AUTHOR (S): Singh, Sanjay K.; Felse, Arthur P.; Nunez, Albertó;

Foglia, Thomas A.; Gross, Richard A.

CORPORATE SOURCE: NSF Center for Biocatalysis and Bioprocessing of

Macromolecules, Department of Chemical Engineering Chemistry and Materials Science, Six Metrotech Center,

Polytechnic University, Brooklyn, NY, 11201, USA

Journal of Organic Chemistry (2003), 68(14), 5466-5477

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER:

American Chemical Society DOCUMENT TYPE:

Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:197675

SOURCE:

AB Novel enzyme-mediated synthetic routes were developed to provide a new family of sophorolipid derivs. and glycolopid-based amphiphilic monomers. These compds. are of great interest for their potential use in immunoregulation, as well as for other biol. properties. In the present work, an efficient lipase-catalyzed conversion of sophorolipid Et ester to (a) the 6'-monoacylated derivs. using Novozym 435, (b) 6''-monoacylated derivs. using Lipase PS-C, (c) secondary amide derivs. using Novozym 435, and (d) 6',6''-diacylated amide derivs. using Novozym 435 in an one-pot reaction and (e) the regioselective monoacylation of an amide derivative at the 6'- and 6''-positions using Novozym 435 and Lipase PS-C, resp., are described. The Et ester produced by esterification of the sophorolipid mixture with sodium ethoxide was subjected to acylation catalyzed by Novozym 435 in dry THF (THF) with vinyl acetate and vinyl methacrylate to produce 6'-monoacylated derivs. In contrast, Lipase PS-C catalyzed acylations of sophorolipid Et ester in dry THF with vinyl acetate and vinyl methacrylate to give the corresponding 6'-monoacylated derivs. Novozym 435 mediated amidation of sophorolipid Et ester in dry THF with phenethylamine, tyramine, p-methoxyphenethylamine, 2-(p-tolyl)ethylamine, and p-fluorophenethylamine generated the corresponding secondary amides but not tertiary amides. The formation of diacyl derivs. of amides was achieved by their treatment with vinyl acetate and vinyl methacrylate in dry THF using Novozym 435 as catalyst. The conversion of sophorolipid Et ester to the same diacyl derivs. of amide (i.e., both amidation and acylation) in high yield was also demonstrated in dry THF by a one-pot reaction using Novozym 435. Furthermore, regioselective monoacylation of a sophorolipid amide at 6' and 6'' in dry THF with vinyl acetate and vinyl methacrylate using Novozym 435 and Lipase PS-C was also demonstrated.

TT 585542-23-0P 585542-24-1P 585542-25-2P 585542-27-4P 585542-28-5P 585542-29-6P 585542-30-9P 585542-31-0P 585542-32-1P 585542-33-2P 585542-34-3P 585542-35-4P 585542-36-5P

RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP

(Preparation)
(regioselective enzyme-catalyzed acylation in synthesis of sophorolipid esters amides and multifunctional monomers)

RN 585542-23-0 HCAPLUS

CN

9-Octadecenoic acid, 17-[(6-0-acetyl-2-0-β-D-glucopyranosyl-β-D-glucopyranosyl)oxy]-, ethyl ester, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 585542-24-1 HCAPLUS CN 9-Octadecenoic acid.

9-Octadecenoic acid, 17-[[2-0-(6-0-acetyl-β-D-glucopyranosyl)-β-D-glucopyranosyl]oxy]-, ethyl ester, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 585542-25-2 HCAPLUS

CN 9-Octadecenoic acid, 17-[[2-O-[6-O-(2-methyl-1-oxo-2-propenyl)- β -D-glucopyranosyl]- β -D-glucopyranosyl]oxy]-, ethyl ester, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 585542-27-4 HCAPLUS

CN 9-Octadecenamide, 17-[(2-0- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-N-(2-phenylethyl)-, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 585542-28-5 HCAPLUS

CN 9-Octadecenamide, 17-[(2-O-β-D-glucopyranosyl-β-Dglucopyranosyl)oxy]-N-[2-(4-methylphenyl)ethyl]-, (9Z,17S)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

HO S R O S
$$(CH_2)$$
 6 Z (CH_2) 7 O HO HO HO HO

RN 585542-29-6 HCAPLUS

CN 9-Octadecenamide, 17-[(2-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-N-[2-(4-methoxyphenyl)ethyl]-, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 585542-30-9 HCAPLUS 9-Octadecenamide, N-[2-(4-fluorophenyl)ethyl]-17-[(2-0- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 585542-31-0 HCAPLUS CN 9-Octadecenamide, 17-[[6-0-acetyl-2-0-(6-0-acetyl- β -D-glucopyranosyl]-N-[2-(4-hydroxyphenyl)ethyl]-, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 585542-32-1 HCAPLUS

CN 9-Octadecenamide, N-[2-(4-hydroxyphenyl)ethyl]-17-[[6-O-(2-methyl-1-oxo-2-propenyl)-2-O-[6-O-(2-methyl-1-oxo-2-propenyl)- β -D-glucopyranosyl]- β -D-glucopyranosyl]oxy]-, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

PAGE 2-A

|| CH₂

RN 585542-33-2 HCAPLUS

CN 9-Octadecenamide, 17-[(6-O-acetyl-2-O-β-D-glucopyranosyl-β-D-glucopyranosyl) oxy] -N-[2-(4-hydroxyphenyl) ethyl]-, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 585542-34-3 HCAPLUS

CN 9-Octadecenamide, 17-[[2-O- β -D-glucopyranosyl-6-O-(2-methyl-1-oxo-2-propenyl)- β -D-glucopyranosyl]oxy]-N-[2-(4-hydroxyphenyl)ethyl]-, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

$$\begin{array}{c} \text{CH}_2 \\ \text{HO} \\ \text{S} \\ \text{R} \\ \text{O} \\ \text{O} \\ \text{S} \\ \text{R} \\ \text{O} \\ \text{O} \\ \text{CH}_2) \\ \text{6} \\ \text{Z} \\ \text{(CH}_2) \\ \text{7} \\ \text{O} \\ \text{O} \\ \text{HO} \\ \text{H$$

RN 585542-35-4 HCAPLUS

9-Octadecenamide, 17-[[2-O-(6-O-acetyl-β-D-glucopyranosyl)-β-Dglucopyranosyl]oxy]-N-[2-(4-hydroxyphenyl)ethyl]-, (9Z,17S)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 585542-36-5 HCAPLUS 9-Octadecenamide, N-[2-(4-hydroxyphenyl)ethyl]-17-[[2-0-[6-0-(2-methyl-1-oxo-2-propenyl)- β -D-glucopyranosyl]- β -D-glucopyranosyl]oxy]-, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

|| CH₂ PAGE 2-A

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

HO S R O Me (CH2)
$$_{6}$$
 $_{2}$ (CH2) $_{7}$ O HO HO HO HO

IT 220608-02-6

RL: RCT (Reactant); RACT (Reactant or reagent)
(regioselective enzyme-catalyzed acylation in synthesis of sophorolipid esters amides and multifunctional monomers)

RN 220608-02-6 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-O-β-D-glucopyranosyl-β-D-glucopyranosyl)oxy]-, ethyl ester, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

REFERENCE COUNT:

61 THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 10 OF 17 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2001:419032 HCAPLUS <<LOGINID::20070809>>

DOCUMENT NUMBER:

135:167087

TITLE:

The synthesis and polymerization of glycolipid-based

monomers

AUTHOR(S):

Bisht, Kirpal S.; Gross, Richard A.

CORPORATE SOURCE:

Center for Biocatalysis and Bioprocessing of Macromolecules, Six Metrotech Center, Polytechnic

University, Brooklyn, NY, 11202, USA

SOURCE:

ACS Symposium Series (2001), 786 (Biopolymers from

Polysaccharides and Agroproteins), 222-239

CODEN: ACSMC8; ISSN: 0097-6156

PUBLISHER: American Chemical Society

DOCUMENT TYPE: LANGUAGE:

Journal English

Well-defined sophorolipid biosurfactant analogs were prepared via enzymic synthesis for evaluation of bioactivity and as building blocks for preparation of glycolipid-based amphiphilic polymers. A 6-0-acryl sophorolipid derivative was prepared and homopolymd. and copolymd. with acrylic acid and acrylamide. The alkyl esters of sophorolipids, produced by Torulopsis bombicola were subjected to Novozym 435 catalyzed acylation in dry THF with vinyl acrylate and vinyl acetate to obtain the diacyl derivs. The regioselective synthesis of 6'-O-acryl sophorolipid derivative was accomplished by a lipase-catalyzed acylation reaction in dry organic solvent. Of the lipases screened, i.e., porcine pancreatic lipase (PPL), Candida rugosa lipase (CCL), PS-30, AK, MAP-10, Novozym-435 and Lipozyme IM, Novozym-435 was the biocatalyst of choice. Subsequent homopolymn. of the C-6' monoacryl sophorolipid derivative and its radical copolymn. with acrylamide and acrylic acid using AIBN afforded glycolipid-containing acrylate polymers.

IT 213754-46-2P 220608-05-9P 220608-09-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; enzymic catalyzed synthesis of sophorolipid acrylate monomer and radical polymerization to obtain glycolipid-based amphiphilic polyacrylates)

RN 213754-46-2 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-O- β -D-glucopyranosyl- β -Dglucopyranosyl)oxy]-, methyl ester, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

MeO (CH₂) 7
$$\underline{Z}$$
 (CH₂) 6 S O OH OH

RN 220608-05-9 HCAPLUS

9-Octadecenoic acid, 17-[[6-0-(1-oxo-2-propenyl)-2-0-[6-0-(1-oxo-2-CN propenyl)- β -D-glucopyranosyl]- β -D-glucopyranosyl]oxy]-, methyl ester, (9Z,17S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 220608-09-3 HCAPLUS

CN 9-Octadecenoic acid, 17-[[6-0-(3-carboxy-1-oxopropyl)-2-0-[6-0-(3-carboxy-

1-oxopropyl) $-\beta$ -D-glucopyranosyl] $-\beta$ -D-glucopyranosyl] oxy] -,

1-methyl ester, (9Z,17S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

$$HO_2C$$
 OH
 O

REFERENCE COUNT:

60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 11 OF 17 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:885905 HCAPLUS <<LOGINID::20070809>>

DOCUMENT NUMBER: 134:206638

TITLE: Production of native and modified sophorose lipids AUTHOR (S): Lang, Siegmund; Brakemeier, Andreas; Heckmann, Rolf;

Spockner, Stefanie; Rau, Udo

CORPORATE SOURCE: Department of Biochemistry and Biotechnology,

Biotechnology Group, Technical University of Braunschweig, Braunschweig, D-38106, Germany

Chimica Oggi (2000), 18(10), 76-79

CODEN: CHOGDS; ISSN: 0392-839X

PUBLISHER: TeknoScienze

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:206638

Depending on the co-substrate, the yeast Candida bombicola is able to

SOURCE:

overproduce different kinds of sophorose lipids during cultivation on glucose as the main carbon and energy source. With oleic acid, yields of 76 g l-1 d-1 were obtained by a continuous process. In contrast to classical products found by this mode, using 2-tetradecanol a novel-type alkyl sophoroside was produced yielding 2.9 g l-1 d-I. The native sophorose lipid first mentioned was modified by a glycosidase-catalyzed reaction to a glucose lipid. Another modification was successfully performed with alkyl amines leading to alkyl amides of the acidic sophorose lipid. Depending on the mol. structure the products reduced the surface tension of water from 72 mN m-1 to a min. of approx. 30 mN m-1 in the case of the 2-tetradecyl sophoroside.

IT 328569-86-4P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(production of native and modified sophorose lipids)

RN 328569-86-4 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-, (9Z)- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

HO
$$\frac{OH}{R}$$
 $\frac{OH}{S}$ $\frac{OH}{$

IT 328569-88-6P 328569-89-7P 328569-90-0P 328569-91-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (production of native and modified sophorose lipids)

RN 328569-88-6 HCAPLUS

CN 9-Octadecenamide, N-butyl-17-[(2-O-β-D-glucopyranosyl-β-D-glucopyranosyl)oxy]-, (9Z)- (9CI) (CA INDEX NAME)

RN 328569-89-7 HCAPLUS

CN 9-Octadecenamide, 17-[(2-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-N-hexyl-, (9Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

Me (CH₂)
$$\frac{H}{S}$$
 (CH₂) $\frac{Z}{S}$ (CH₂) $\frac{C}{S}$ (CH₂) $\frac{Z}{S}$ (CH₂)

RN 328569-90-0 HCAPLUS

CN 9-Octadecenamide, N-decyl-17-[(2-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-, (9Z)- (9ZI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

Me (CH₂)
$$\frac{H}{9}$$
 (CH₂) $\frac{Z}{0}$ (CH₂)

RN 328569-91-1 HCAPLUS

CN 9-Octadecenamide, 17-[(2-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-N-(1-methylpropyl)-, (9Z)- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 12 OF 17 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1999:810168 HCAPLUS <<LOGINID::20070809>>

DOCUMENT NUMBER:

132:136455

TITLE:

Enzymatic conversion of a sophorolipid into a glucose

lipid

English

AUTHOR (S):

SOURCE:

CORPORATE SOURCE:

Rau, Udo; Heckmann, Rolf; Wray, Victor; Lang, Siegmund Institut fur Biochemie und Biotechnologie, Technische

Universitat Braunschweig, Braunschweig, 38106, Germany Biotechnology Letters (1999), 21(11), 973-977

CODEN: BILED3; ISSN: 0141-5492

PUBLISHER: Kluwer Academic Publishers Journal

DOCUMENT TYPE: LANGUAGE:

OTHER SOURCE(S): CASREACT 132:136455

The diacetylated lactonic sophorolipid from Candida bombolica was converted into the deacetylated acidic form by alkaline hydrolysis and subsequently treated with several glycosidases. One of these enzymes, a hesperidinase (E.C. 3.2.1.40), was most active in the specific release of one glucose mol. from the disaccharide lipid. The novel glucolipid was isolated and characterized. The surface and interfacial tension of aqueous solns. were measured and compared with the lactonic and acidic sophorolipid.

IT 220608-11-7

RL: BPR (Biological process); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); PROC (Process); RACT (Reactant or reagent)

(enzymic conversion of a sophorolipid into a glucose lipid)

RN 220608-11-7 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-O- β -D-glucopyranosyl- β -Dglucopyranosyl)oxy]-, (9Z,17S)- (9CI) (CA INDEX NAME)

HO
$$\frac{OH}{R}$$
 $\frac{OH}{R}$ $\frac{OH}{$

REFERENCE COUNT: THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 13 OF 17 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:29511 HCAPLUS <<LOGINID::20070809>>

DOCUMENT NUMBER:

130:182663

TITLE:

Enzyme-Mediated Regioselective Acylations of

Sophorolipids

AUTHOR (S):

Bisht, Kirpal S.; Gross, Richard A.; Kaplan, David L.

CORPORATE SOURCE: SOURCE:

Polytechnic University, Brooklyn, NY, 11201, USA

Journal of Organic Chemistry (1999), 64(3), 780-789 CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER:

American Chemical Society

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 130:182663

Enzymic synthesis of well-defined sophorolipid analogs for evaluation of their bioactivities and as new building blocks for the preparation of glycolipid-based amphiphilic polymers is described. Lipase Novozym 435 from Candida antarctica has been shown to be an efficient catalyst for acylation of sophorolipids esters. A mixture of sophorolipids produced by Torulopsis bombicola was esterified by reaction with sodium alkoxide. The alkyl esters of sophorose lipids were subjected to Novozym 435 catalyzed acylation in dry THF with vinyl acrylate and vinyl acetate to diacyl derivs. The reactions were highly regioselective, and exclusive acylation of the hydroxyl groups on C-6' and C-6'' took place. Me ester in the absence of the acylating agent, or with the agent at a concentration less than equimolar, gave sophorolactone. Careful anal. of the spectral data revealed it to be a synthetic analog of microbially produced macrolactone. Sophorolactone differs in the site at which the sophorose ring is attached to the fatty acid. Specifically, unlike the natural sophorolipids, the fatty acid carboxyl carbon is linked to the C-6'' hydroxyl, not to the C-4'' hydroxyl. Subsequent acrylation catalyzed by Novozym 435 led to the formation of the C-6' monoacryl derivative linked only to the primary site. IT 220608-05-9P 220608-06-0P 220608-07-1P

220608-08-2P 220608-09-3P

RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)

(enzyme-mediated regioselective acylations of sophorolipids)

RN220608-05-9 HCAPLUS

CN9-Octadecenoic acid, 17-[[6-0-(1-oxo-2-propenyl)-2-0-[6-0-(1-oxo-2propenyl)- β -D-glucopyranosyl]- β -D-glucopyranosyl]oxy]-, methyl ester, (9Z,17S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 220608-06-0 HCAPLUS

CN 9-Octadecenoic acid, 17-[[6-O-acetyl-2-O-(6-O-acetyl- β -D-glucopyranosyl)- β -D-glucopyranosyl]-, methyl ester, (9Z,17S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 220608-07-1 HCAPLUS

CN 9-Octadecenoic acid, 17-[[6-O-acetyl-2-O-(6-O-acetyl- β -D-glucopyranosyl)- β -D-glucopyranosyl]oxy]-, ethyl ester, (9Z,17S)-(9CI) (CA INDEX NAME)

RN 220608-08-2 HCAPLUS
CN 9-Octadecenoic acid, 17-[[6-O-acetyl-2-O-(6-O-acetyl-β-D-glucopyranosyl)-β-D-glucopyranosyl]oxy]-, butyl ester, (9Z,17S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 220608-09-3 HCAPLUS

CN 9-Octadecenoic acid, 17-[[6-0-(3-carboxy-1-oxopropyl)-2-0-[6-0-(3-carboxy-1-oxopropyl)-β-D-glucopyranosyl]-β-D-glucopyranosyl]οxy]-,

1-methyl ester, (9Z,17S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

$$HO_2C$$
 OH
 O

IT 220608-11-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(enzyme-mediated regioselective acylations of sophorolipids)

RN 220608-11-7 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-0- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

IT 213754-46-2P 220608-02-6P 220608-04-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (enzyme-mediated regioselective acylations of sophorolipids)
RN 213754-46-2 HCAPLUS
CN 9-Octadecenoic acid, 17-[(2-O-β-D-glucopyranosyl-β-D-glucopyranosyl)oxy]-, methyl ester, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 220608-02-6 HCAPLUS CN 9-Octadecenoic acid, 17-[(2-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-, ethyl ester, (9Z,17S)- (9CI) (CA INDEX NAME)

RN 220608-04-8 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-O- β -D-glucopyranosyl- β -D-

glucopyranosyl)oxy]-, butyl ester, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

REFERENCE COUNT:

50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 14 OF 17 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1998:546435 HCAPLUS <<LOGINID::20070809>>

DOCUMENT NUMBER:

129:276158

TITLE:

Glycolipid containing polyacrylate and polyacrylamide

copolymers

AUTHOR(S):

Bisht, Kirpal; Watterson, Arthur C.; Gross, Richard A.

CORPORATE SOURCE:

Dep. Chem., Univ. Massachusetts, Lowell, MA, 01854,

USA

SOURCE:

Polymeric Materials Science and Engineering (1998),

79, 246-247

CODEN: PMSEDG; ISSN: 0743-0515

PUBLISHER:

American Chemical Society

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB Enzymic transformations were carried out on sophorose lipid, produced by T. bombicola grown on a mixture of oleic acid and glucose, in a regio-specific manner. Homo- or co-polymerization, with acrylic acid or acrylamide, was undertaken to produce polymer structures bearing amphiphilic side chain groups, which have potential for use as pharmacol. active agents.

IT 213754-46-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(glycolipid-containing polyacrylate and polyacrylamide copolymers)

RN 213754-46-2 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-O- β -D-glucopyranosyl- β -D-

glucopyranosyl)oxy]-, methyl ester, (9Z,17S)- (9CI) (CA INDEX NAME)

MeO (CH₂) 7
$$\underline{Z}$$
 (CH₂) 6 S O OH

REFERENCE COUNT:

5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 15 OF 17 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

DOCUMENT NUMBER:

129:285646

TITLE:

Bioactivity of extracellular glycolipids -

investigation of potential anti-cancer activity of

sophorolipids and sophorolipid-derivatives

AUTHOR (S):

Scholz, C.; Mehta, S.; Bisht, K.; Guilmanov, V.;

Kaplan, D.; Nicolosi, R.; Gross, R.

CORPORATE SOURCE:

Department of Chemistry, University of Massachusetts,

Lowell, MA, 01854, USA

SOURCE:

Polymer Preprints (American Chemical Society, Division

of Polymer Chemistry) (1998), 39(2), 168-169

CODEN: ACPPAY; ISSN: 0032-3934

PUBLISHER:

American Chemical Society, Division of Polymer

Chemistry

DOCUMENT TYPE:

Journal

LANGUAGE: English

Sophorolipid (SL) analogs were prepared by alcoholysis and enzyme-catalyzed acetylation of a complex natural SL-mixture of Candida bombicola obtained from fermentation The extent was determined of Jurkat (leukemia) and Tu 138 (head and neck cancer) cell growth inhibition resulting from exposure of the cells to different SL-analogs. Acetylation at the primary positions of the SL carbohydrate head group showed a potential anticancer activity for both cancer cell lines. The Tu 138 cell line seemed to be more susceptible than the Jurkat cells to treatment with the SL-derivs. 138 cell line showed enhanced inhibition of cell growth by increasing the chain length from C4 to C10 of the n-alkanol that was esterified to the SL lipid moiety.

IT 214218-57-2P 214218-58-3P 214218-59-4P

214218-60-7P 214218-61-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological

study); PREP (Preparation)

(potential anti-cancer activity of sophorolipids and sophorolipid-derivs.)

RN 214218-57-2 HCAPLUS

9-Octadecenoic acid, 17-[(2-O-β-D-glucopyranosyl-β-D-CN glucopyranosyl)oxy]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

RN 214218-58-3 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-, butyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 214218-59-4 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-O-β-D-glucopyranosyl-β-D-glucopyranosyl)oxy]-, decyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

Me
$$(CH_2)_9$$
 OH $(CH_2)_7$ OH $(CH_2)_6$ OH

RN 214218-60-7 HCAPLUS

CN 9-Octadecenoic acid, 17-[[6-0-acetyl-2-0-(6-0-acetyl- β -D-glucopyranosyl)- β -D-glucopyranosyl]oxy]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 214218-61-8 HCAPLUS

CN 9-Octadecenoic acid, 17-[[6-O-acetyl-2-O-(6-O-acetyl-β-D-glucopyranosyl)-β-D-glucopyranosyl]oxy]-, butyl ester (9CI) (CFINDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

REFERENCE COUNT:

3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 16 OF 17 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1997:396246 HCAPLUS <<LOGINID::20070809>>

DOCUMENT NUMBER:

127:120735

TITLE:

A sophorose lipid from microbial conversion of oleyl

alcohol

AUTHOR (S):

Shi, Yi Ping; Li, Jiang Yun; Li, Zu Yi

CORPORATE SOURCE:

State Key Lab. Bioorg. Natural Product Chem., Shanghai Inst. Org. Chem., Shanghai, 200032, Peop. Rep. China

Chinese Chemical Letters (1997), 8(5), 417-418

CODEN: CCLEE7

PUBLISHER:

SOURCE:

Chinese Chemical Society

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB Using oleyl alc. as C source for the cultivation of yeast Torulopsis sp., a modified sophorose lipid was isolated as the major product. This product was characterized as the octadecyl derivative by 1H NMR and FAB-MS. Hydrogenation gave an octadecyl ester: octadecyl 17-L-[(2'-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy] octadecanoate 6',6'-diacetate. IT 192811-02-2P

(sophorose lipid from microbial conversion of oleyl alc.)

RN 192811-02-2 HCAPLUS

CN 9-Octadecenoic acid, 17-[[6-O-acetyl-2-O-(6-O-acetyl-β-D-glucopyranosyl)-β-D-glucopyranosyl]oxy]-, (9Z)-9-octadecenyl ester, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

PAGE 1-A

Me (CH₂)
$$7$$
 Z (CH₂) 8 O (CH₂) 7 Z (CH₂) 6 S O Me

PAGE 1-B

REFERENCE COUNT:

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 17 OF 17 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1995:796820 HCAPLUS <<LOGINID::20070809>>

DOCUMENT NUMBER: 123:250351
TITLE: Tandem mass

Tandem mass spectrometry and nuclear magnetic

resonance spectroscopy studies of Candida bombicola sophorolipids and product formed on hydrolysis by

cutinase

AUTHOR(S): de Koster, Chris G.; Heerma, Wigger; Pepermans, Henri

A. M.; Groenewegen, Anneke; Peters, Hans; Haverkamp,

Johan

CORPORATE SOURCE: Bijvoet Center for Biomolecular Research, Univ.

Utrecht, Utrecht, 3508 TB, Neth.

Analytical Biochemistry (1995), 230(1), 135-48 SOURCE:

CODEN: ANBCA2; ISSN: 0003-2697

PUBLISHER: Academic DOCUMENT TYPE: Journal LANGUAGE: English

Natural mixts. of sophorolipids produced by the yeast Candida bombicola have been analyzed by fast-atom-bombardment (FAB)-MS and collision-induced dissociation (CID)-MS. Some pure components were analyzed by 2-dimensional NMR spectroscopy. The presence of acidic, lactonic, and O-acetylated forms and the position of double bonds in the fatty acid part of these glycolipids can be easily inferred from pos. - and neq. -ion FAB-mass spectra. Details about position of O-acetylation can be obtained from CID mass spectra of [M + H] + and [M - H] - ions and from the NMR spectra. Differences in CID fragmentation between protonated and sodiated mol. ions are discussed in detail. Enzymic hydrolysis of 6',6''-di-0-acetyl sophorolipid lactone by cutinase from Fusarium solani results specifically in the removal of the 6'-O-acetyl group, whereas the 6''-O-acetyl and lactone group are resistant. This specificity is explained from a 3-dimensional model of the sophorolipid generated on the basis of the short 1H,1H distances as inferred from the NMR (ROESY) spectra.

IT 168699-93-2 168699-96-5 168699-97-6

168699-99-8

RL: ANT (Analyte); PRP (Properties); ANST (Analytical study) (tandem mass spectrometry and NMR spectroscopy of Candida sophorolipids and cutinase hydrolysis product)

RN 168699-93-2 HCAPLUS

CN 8-Heptadecenoic acid, 16-[(2-0-β-D-glucopyranosyl-Dglucopyranosyl)oxy]-, (Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

HO
$$_{\rm HO_{2}C}$$
 OH $_{\rm R}$ S $_{\rm S}$ OH $_{\rm R}$ S $_{\rm S}$ OH $_{\rm OH}$ OH $_{\rm HO_{2}C}$ OH $_{\rm Me}$

RN168699-96-5 HCAPLUS

CN 8-Heptadecenoic acid, 16-[[2-0-(6-0-acetyl-β-D-glucopyranosyl)-Dglucopyranosyl]oxy]-, (Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

HO
$$\frac{OH}{R}$$
 $\frac{OH}{S}$ $\frac{OH}{R}$ $\frac{OH}{S}$ $\frac{OH}{$

RN 168699-97-6 HCAPLUS

CN 8-Heptadecenoic acid, 16-[(6-0-acetyl-2-0- β -D-glucopyranosyl-D-glucopyranosyl)oxy]-, (Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 168699-99-8 HCAPLUS

CN 8-Heptadecenoic acid, 16-[[6-0-acetyl-2-0-(6-0-acetyl-β-D-glucopyranosyl)-D-glucopyranosyl]oxy]-, (Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

ACO R S OH OAC OH
$$R$$
 S R OH R OH

=> fil stng
COST IN U.S. DOLLARS

SINCE FILE

TOTAL

```
Uploading C:\Program Files\Stnexp\Queries\778ii.str
```

chain nodes : 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 ring nodes : 1 2 3 4 5 6 7 8 9 10 11 12 chain bonds : 1-21 2-13 4-24 5-23 6-22 7-14 9-25 10-19 11-20 12-13 14-15 15-16 15-17 16-18 18-28 24-26 25-27 28-29 29-30 30-31 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 exact/norm bonds : 1-2 1-6 1-21 2-3 2-13 3-4 4-5 5-6 5-23 6-22 7-8 7-12 7-14 8-9 9-10 10-11 10-19 11-12 11-20 12-13 14-15 24-26 25-27 30-31 exact bonds : 4-24 9-25 15-16 15-17 16-18 18-28 28-29 29-30

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS

L1 STRUCTURE UPLOADED

=> s l1 sss sam

SAMPLE SEARCH INITIATED 16:14:57 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 876 TO ITERATE

100.0% PROCESSED 876 ITERATIONS 4 ANSWERS SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 15745 TO 19295
PROJECTED ANSWERS: 4 TO 200

L2 4 SEA SSS SAM L1

=> d scan

L2 4 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 9-Octadecenamide, 17-[(2-O-β-D-glucopyranosyl-β-D-glucopyranosyl)oxy]-N-[2-(4-methoxyphenyl)ethyl]-, (9Z,17S)- (9CI)

MF C39 H65 N O13

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):4

L2 4 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN L-Glutamic acid, N-[(9Z)-17-[(2-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-1-oxo-9-octadecen-1-yl]-, 1,5-bis(1,1-dimethylethyl) ester

MF C43 H77 N O16

Absolute stereochemistry. Double bond geometry as shown.

PAGE 1-A

PAGE 1-B

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 4 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN INDEX NAME NOT YET ASSIGNED

MF C32 H56 O14

Absolute stereochemistry. Double bond geometry unknown.

HO
$$\frac{OH}{R}$$
 $\frac{OH}{S}$ $\frac{OH}{$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 4 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

9-Octadecenamide, 17-[(2-O- β -D-glucopyranosyl- β -D-IN

glucopyranosyl)oxy]-N-hexyl-, (9Z)- (9CI) C36 H67 N O12

MF

Absolute stereochemistry. Double bond geometry as shown.

Me (CH₂)
$$\frac{H}{5}$$
 (CH₂) $\frac{Z}{5}$ (CH₂)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> s l1 sss full FULL SEARCH INITIATED 16:15:12 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 18133 TO ITERATE

100.0% PROCESSED 18133 ITERATIONS

68 ANSWERS

SEARCH TIME: 00.00.01

L3 68 SEA SSS FUL L1

=> fil hcaplus COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 172.10 173.36

FULL ESTIMATED COST

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=> s 13

L4 21 L3

```
=> s virus or antiviral or HIV
        366796 VIRUS
        77485 VIRUSES
        380559 VIRUS
                 (VIRUS OR VIRUSES)
         61195 ANTIVIRAL
         1228 ANTIVIRALS
         61442 ANTIVIRAL
                 (ANTIVIRAL OR ANTIVIRALS)
         73360 HIV
            98 HIVS
         73377 HIV
                 (HIV OR HIVS)
L5
        415133 VIRUS OR ANTIVIRAL OR HIV
=> s 14 and 15
             4 L4 AND L5
L6
=> d 16 ibib abs hitstr 1-4
     ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:
                         DOCUMENT NUMBER:
                         146:41746
                         Amino Acid Conjugated Sophorolipids: A New Family of
TITLE:
                         Biologically Active Functionalized Glycolipids
AUTHOR(S):
                         Azim, Abul; Shah, Vishal; Doncel, Gustavo F.;
                         Peterson, Nicholas; Gao, Wei; Gross, Richard
CORPORATE SOURCE:
                         NSF I/UCR Center for Biocatalysis and Bioprocessing of
                         Macromolecules, Polytechnic University, Brooklyn, NY,
                         11201, USA
                         Bioconjugate Chemistry (2006), 17(6), 1523-1529
SOURCE:
                         CODEN: BCCHES; ISSN: 1043-1802
PUBLISHER:
                         American Chemical Society
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                         English
     Sophorolipids (SLs) are extra cellular glycolipids produced by Candida
     bombicola ATCC 22214 when grown in the presence of glucose and fatty
            These compds. have a disaccharide head group connected to a
     long-chain hydroxyl-fatty acid by a glycosidic bond. To explore
     structure-activity of modified SLs, a new family of amino acid-SL derivs.
     was prepared Synthesized analogs consist of amino acids linked by amide
     bonds formed between their \alpha-amino moiety and the carboxyl group of
     ring-opened SL fatty acids. Their preparation involved the following: (i)
     hydrolysis of a natural SL mixture with aqueous alkali to give SL free acids,
     (ii) coupling of free acids to protected amino acids using dicarbodiimide,
     and (iii) removing amino acid carboxyl protecting groups. These
     conjugates were evaluated for their antibacterial, anti-HIV, and
     spermicidal activity. All tested analogs showed antibacterial activity
     against both gram pos. and gram neg. organisms. Leucine-conjugated SL was
     most efficient. For example, the min. inhibitory concns. (MIC) for
     Moraxella sp. and E. coli were 0.83 and 1.67 mg/mL, resp.
                                                               Among the alkyl
     esters of amino acid conjugated SLs, the Et ester of leucine-SLs was most
     active. Against Moraxella sp., S. sanguinis, and M. imperiale, MIC values
     are 7.62+10-4, 2.28+10-3 and 1.67 mg/mL, resp. All compds.
     displayed virus-inactivating activity with 50% effective concns.
     (EC50) below 200 μg/mL. The EC50 of leucine-SL Et ester was 24.1
     μg/mL, showing that it is more potent than com. spermicide nonoxynol-9
     (EC50 \approx 65 \mug/mL).
TT
     916601-59-7P 916601-61-1P 916601-64-4P
     916601-65-5P 916601-66-6P
     RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);
     BIOL (Biological study); PREP (Preparation)
```

(synthesis of amino acid-conjugated sophorolipids)

RN 916601-59-7 HCAPLUS

CN L-Glutamic acid, N-[(9Z)-17-[(2-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-1-oxo-9-octadecen-1-yl]- (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

PAGE 1-B

→ OH

....ОН

RN 916601-61-1 HCAPLUS

CN L-Serine, N-[(9Z)-17-[(2-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-1-oxo-9-octadecen-1-yl]- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

HO S N (CH2) 7 Z (CH2) 6 O OH

$$CO_{2}H$$
 O $CO_{2}H$ O $CO_{2}H$

RN 916601-64-4 HCAPLUS

CN L-Phenylalanine, N-[(9Z)-17-[(2-O-β-D-glucopyranosyl-β-D-glucopyranosyl)oxy]-1-oxo-9-octadecen-1-yl]-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 916601-65-5 HCAPLUS
CN L-Leucine, N-[(9Z)-17-[(2-O-β-D-glucopyranosyl-β-D-glucopyranosyl)oxy]-1-oxo-9-octadecen-1-yl]-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 916601-66-6 HCAPLUS

CN Glycine, N-[(9Z)-17-[(2-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-1-oxo-9-octadecen-1-yl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

MeO
$$(CH_2)_7$$
 Z $(CH_2)_6$ OH OH OH OH Me

IT 328569-86-4

RL: RCT (Reactant); RACT.(Reactant or reagent) (synthesis of amino acid-conjugated sophorolipids)

RN 328569-86-4 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxyl-, (9Z)- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

Absolute stereochemistry.

Double bond geometry as shown.

RN 916601-55-3 HCAPLUS
CN L-Serine, N-[(9Z)-17-[(2-0-β-D-glucopyranosyl-β-D-glucopyranosyl)oxy]-1-oxo-9-octadecen-1-yl]-, phenylmethyl ester (CI INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

PAGE 1-B

◯OH

`...ОН

RN 916601-56-4 HCAPLUS CN L-Leucine, N-[(9Z)-17-[(2-O- β -D-glucopyranosyl- β -D-

glucopyranosyl)oxy]-1-oxo-9-octadecen-1-yl]-, phenylmethyl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 916601-57-5 HCAPLUS

CN L-Phenylalanine, N-[(9Z)-17-[(2-O-β-D-glucopyranosyl-β-D-glucopyranosyl)oxy]-1-oxo-9-octadecen-1-yl]-, phenylmethyl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

PAGE 1-B

_OH

....ОН

RN 916601-58-6 HCAPLUS

CN L-Glutamic acid, N-[(9Z)-17-[(2-O- β -D-glucopyranosyl- β -D-

glucopyranosyl)oxy]-1-oxo-9-octadecen-1-yl]-, 1,5-bis(1,1-dimethylethyl)

ester (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

PAGE 1-A

t-BuO
$$(CH_2)$$
 7 Z (CH_2) 6 O Me

PAGE 1-B

REFERENCE COUNT:

19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:1093774 HCAPLUS <<LOGINID::20070809>>

DOCUMENT NUMBER: 144:3139

TITLE: Sophorolipids, microbial glycolipids with anti-human

immunodeficiency virus and sperm-immobilizing activities

AUTHOR(S): Shah, Vishal; Doncel, Gustavo F.; Seyoum, Theodoros;

Eaton, Kristin M.; Zalenskaya, Irina; Hagver, Rena;

Azim, Abul; Gross, Richard

CORPORATE SOURCE: NSF Center for Biocatalysis and Bioprocessing of

Macromolecules, Six Metrotech Center, Polytechnic

University, Brooklyn, NY, 11201, USA

SOURCE: Antimicrobial Agents and Chemotherapy (2005), 49(10),

4093-4100

CODEN: AMACCQ; ISSN: 0066-4804

PUBLISHER: American Society for Microbiology

DOCUMENT TYPE:

Journal

LANGUAGE: English AΒ The increased incidence of human immunodeficiency virus (HIV)/AIDS disease in women aged 15 to 49 years has identified the urgent need for a female-controlled, efficacious, and safe vaginal topical microbicide. To meet this challenge, sophorolipid (SL) produced by Candida bombicola and its structural analogs have been studied in this report for their spermicidal, anti-HIV, and cytotoxic activities. The sophorolipid diacetate Et ester derivative is the most potent spermicidal and virucidal agent of the series of SLs studied. Its virucidal activity against HIV and sperm-immobilizing activity against human semen are similar to those of nonoxynol-9. However, it also induced enough vaginal cell toxicity to raise concerns about its applicability for long-term microbicidal contraception. Its structure-activity relationship has been established for creating new analogs with less cytotoxicity and higher activity.

IT 213754-46-2 220608-02-6 220608-07-1 220608-11-7 585542-23-0 693786-10-6 777091-27-7 799796-29-5 870150-68-8

RL: BSU (Biological study, unclassified); BIOL (Biological study) (sophorolipids, microbial glycolipids with anti-human immunodeficiency virus and sperm-immobilizing activities)

RN 213754-46-2 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-0- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-, methyl ester, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

MeO (CH₂) 7
$$Z$$
 (CH₂) 6 S O OH OH

RN 220608-02-6 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-, ethyl ester, (9Z,17S)- (9CI) (CA INDEX NAME)

RN 220608-07-1 HCAPLUS

CN 9-Octadecenoic acid, 17-[[6-O-acetyl-2-O-(6-O-acetyl- β -D-glucopyranosyl)- β -D-glucopyranosyl]oxy]-, ethyl ester, (9Z,17S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 220608-11-7 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

HO
$$_{\rm R}$$
 $_{\rm R}$ $_{\rm C}$ $_{\rm CH_2}$ $_{\rm CH_2}$ $_{\rm C}$ $_{\rm CH_2}$ $_{\rm CH_2}$

RN 585542-23-0 HCAPLUS

CN 9-Octadecenoic acid, 17-[(6-O-acetyl-2-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-, ethyl ester, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 693786-10-6 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-, hexyl ester, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

Me (CH₂)
$$\frac{OH}{S}$$
 (CH₂) $\frac{Z}{S}$ (CH₂) $\frac{CH_2}{S}$ $\frac{Z}{S}$ (CH₂) $\frac{A}{S}$ $\frac{CH_2}{S}$ $\frac{A}{S}$ $\frac{CH_2}{S}$ $\frac{A}{S}$ $\frac{CH_2}{S}$ $\frac{A}{S}$ $\frac{CH_2}{S}$ $\frac{A}{S}$ $\frac{CH_2}{S}$ $\frac{A}{S}$ $\frac{A}{S}$ $\frac{CH_2}{S}$ $\frac{A}{S}$ $\frac{A}{S}$ $\frac{CH_2}{S}$ $\frac{A}{S}$ \frac{A}

RN 777091-27-7 HCAPLUS

CN 9-Octadecenoic acid, 17-[[6-O-acetyl-2-O-(6-O-acetyl- β -D-glucopyranosyl]- β -D-glucopyranosyl]-, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

ACO R S OH OH OH OH HO2C
$$(CH_2)$$
 7 Z (CH_2) 6 S O OH OH

RN 799796-29-5 HCAPLUS

CN 9-Octadecenoic acid, 17-[[2-O-(6-O-acetyl- β -D-glucopyranosyl)- β -D-glucopyranosyl]oxy]-, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

HO
$$\frac{OH}{R}$$
 $\frac{OH}{S}$ $\frac{OH}{$

RN 870150-68-8 HCAPLUS

CN 9-Octadecenoic acid, 17-[(6-0-acetyl-2-0- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

ACO R S OH OH OH OH HO₂C
$$(CH_2)$$
 7 Z (CH_2) 6 S O OH OH

REFERENCE COUNT:

35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:
                              DOCUMENT NUMBER:
                              142:22342
TITLE:
                              Spermicidal and virucidal properties of various forms
                              of sophorolipids produced by Candida bombicola
INVENTOR(S):
                              Gross, Richard A.; Shah, Vishal; Doncel, Gustavo F.
PATENT ASSIGNEE(S):
                              USA
SOURCE:
                              U.S. Pat. Appl. Publ., 9 pp.
                              CODEN: USXXCO
DOCUMENT TYPE:
                              Patent
LANGUAGE:
                              English
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
      PATENT NO.
                            KIND
                                    DATE
                                                  APPLICATION NO.
                                                                                DATE
                                                    -----
                                      20041202
      US 2004242501
                              A1
                                                    US 2004-804778
                                                                                20040319
      CA 2559808
                              A1
                                      20050929
                                                    CA 2005-2559808
                                                                                20050318
      WO 2005089522
                              A2
                                      20050929
                                                    WO 2005-US9486
                                                                                20050318
      WO 2005089522
                              A3
                                      20070329
           W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
          CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, US RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                CN, ;CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
      EP 1750726
                              A2
                                      20070214
                                                  EP 2005-733074
                                                                                20050318
               AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
                IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA,
               HR, LV, MK, YU
PRIORITY APPLN. INFO.:
                                                    US 2003-456208P
                                                                           P 20030320
                                                    US 2004-804778
                                                                            A 20040319
                                                     WO 2005-US9486
                                                                           W 20050318
AB
      A method for producing sophorolipids having spermicidal and/or
      antiviral properties by synthesizing the sophorolipid by fermentation of
      Candida bombicola in a fermentation media to form a natural mixture of lactonic
      sophorolipids compds. and non-lactonic sophorolipids compds. and utilizing
      the natural mixture as a spermicidal and/or antiviral agent,
      and/or separating the lactonic sophorolipids from the natural mixture to form a
      lactonic fraction and mixing all remaining fractions to form a
      non-lactonic fraction and utilizing the lactonic fraction and/or the
      non-lactonic fraction as an spermicidal and/or antiviral agent,
      and sophorolipid compds. for use as spermicidal and/or antiviral
      agents.
IT
      220608-07-1P
      RL: BCP (Biochemical process); IMF (Industrial manufacture); PUR
      (Purification or recovery); RCT (Reactant); BIOL (Biological study); PREP
      (Preparation); PROC (Process); RACT (Reactant or reagent)
          (spermicidal and virucidal properties of various forms of sophorolipids
         produced by Candida bombicola)
RN
      220608-07-1 HCAPLUS
CN
      9-Octadecenoic acid, 17-[[6-0-acetyl-2-0-(6-0-acetyl-β-D-
      glucopyranosyl)-\beta-D-glucopyranosyl]oxy]-, ethyl ester, (92,178)-
      (9CI)
             (CA INDEX NAME)
```

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.

IT 777091-27-7P

> RL: BMF (Bioindustrial manufacture); CPS (Chemical process); PEP (Physical, engineering or chemical process); PUR (Purification or recovery); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)

(spermicidal and virucidal properties of various forms of sophorolipids produced by Candida bombicola)

RN 777091-27-7 HCAPLUS

CN 9-Octadecenoic acid, 17-[[6-O-acetyl-2-O-(6-O-acetyl-β-Dglucopyranosyl) - β -D-glucopyranosyl] oxyl -, (9Z,17S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

ACO R S OH OH OH OH HO2C
$$(CH_2)$$
 7 Z (CH_2) 6 S O OH OH

IT 220608-02-6P 220608-11-7P 693786-10-6P

RL: BMF (Bioindustrial manufacture); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(spermicidal and virucidal properties of various forms of sophorolipids produced by Candida bombicola)

220608-02-6 HCAPLUS RN

CN 9-Octadecenoic acid, 17-[(2-O-β-D-glucopyranosyl-β-Dglucopyranosyl)oxy]-, ethyl ester, (9Z,17S)- (9CI) (CA INDEX NAME)

RN 220608-11-7 HCAPLUS CN 9-Octadecenoic acid, 17-[(2-O- β -D-glucopyranosyl- β -D-

glucopyranosyl)oxy]-, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

HO₂C
$$(CH_2)_7$$
 Z $(CH_2)_6$ S O OH OH

RN 693786-10-6 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-, hexyl ester, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

Me (CH2) 5
$$O$$
 (CH2) 7 Z (CH2) 6 S O OH C

RN .799796-29-5 HCAPLUS

CN 9-Octadecenoic acid, $17-[[2-0-(6-0-acetyl-\beta-D-glucopyranosyl)-\beta-$ D-glucopyranosyl]oxy]-, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

HO
$$\frac{OH}{R}$$
 $\frac{OH}{S}$ $\frac{OH}{R}$ $\frac{OH}{S}$ $\frac{OH}{$

ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

DOCUMENT NUMBER:

141:5877

TITLE:

Antimicrobial properties of various forms of

sophorolipids

INVENTOR(S):

Gross, Richard A.; Shah, Vishal

PATENT ASSIGNEE(S): SOURCE:

Polytechnic University, USA PCT Int. Appl., 40 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent English

LANGUAGE: FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.					KIND DATE			APPLICATION NO.									
WO 2004044216								WO 2003-US35871									
W									BA, BB, BG, BR, BY,								
•		, CR,															
		HR,															
		, LT,															
	TD.	, PH,	PL,	PI,	RO,	KU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	TJ,	TM,	TN,	
ъ.	IK.	, TT,	12,	UA,	UG,	US,	UZ,	VC,	VN,	ΥU,	ZA,	ZM,	ZW				
R	W: BW																
		, KG,															
	ES	, FI,	FR,	GB,	GR,	HU,	ΙE,	IT,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	SK,	
	, TR	, BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG
AU 2003299557			A1	11 20040603				AU 2003-299557					20031106				
				1 20050728				US 2004-20683									
WO 2006069175			A2		2006	0629	WO 2005-US46426						20051222				
WO 2006069175													_				
W	: AE	, AG,	AL,	AM,	ΑT,	AU,	ΑZ,	BA,	BB,	ВĠ,	BR,	BW,	BY,	BZ,	CA,	CH,	
•		, co,															
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	SG	sK,	SL,	SM.	SY.	TJ.	TM.	TN.	TR.	TT.	TZ.	IIA .	UG.	US.	117.	VC	
		YU,				•	, . ,	,		,	,	/	7	55,	,	,	
RI	V: AT		•	•		CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	

IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.:

US 2002-424271P P 20021106 WO 2003-US35871 W 20031106 US 2004-20683 A2 20041222

The preparation and use of $17-L-[(2'-O-\beta-D-glucopyranosyl-\beta-D-glucopyranosyl) oxy]-cis-9-octadecenoate, lactonic and open ring <math>17-L-[(2'-O-\beta-D-glucopyranosyl-\beta-D-glucopyranosyl) oxy]-cis-9-octadecenoate, Me <math>17-L-[(2'-O-\beta-D-glucopyranosyl-\beta-D-glucopyranosyl) oxy]-cis-9-octadecenoate, Et <math>17-L-[(2'-O-\beta-D-glucopyranosyl-\beta-D-glucopyranosyl) oxy]-cis-9-octadecenoate, hexyl <math>17-L-[(2'-O-\beta-D-glucopyranosyl-\beta-D-glucopyranosyl) oxy]-cis-9-octadecenoate, Et <math>17-L-[(2'-O-\beta-D-glucopyranosyl-\beta-D-glucopyranosyl) oxy]-cis-9-octadecenoate, Et <math>17-L-[(2'-O-\beta-D-glucopyranosyl-\beta-D-glucopyranosyl) oxy]-cis-9-octadecenoate-6',6''-diacetate sophorolipids are antibacterial, antiviral and/or anti-spermicidal agents.$

IT 213754-46-2P 220608-02-6P

RL: BPN (Biosynthetic preparation); BSU (Biological study, unclassified); IMF (Industrial manufacture); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)

(antimicrobial properties of various forms of sophorolipids)

RN 213754-46-2 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-0- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-, methyl ester, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

MeO
$$(CH_2)_7$$
 Z $(CH_2)_6$ S O OH OH

RN 220608-02-6 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-, ethyl ester, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 585542-24-1 HCAPLUS

CN 9-Octadecenoic acid, 17-[[2-0-(6-0-acetyl-β-D-glucopyranosyl)-β-D-glucopyranosyl]oxy]-, ethyl ester, (9Z,17S)- (9CI) (CA INDEX NAME)

RN 693786-10-6 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-, hexyl ester, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

Me (CH₂)
$$\frac{OH}{S}$$
 (CH₂) $\frac{CH_2}{S}$ $\frac{CH_2}{S}$

IT 220608-11-7P

RL: BPN (Biosynthetic preparation); BSU (Biological study, unclassified); IMF (Industrial manufacture); PUR (Purification or recovery); RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(antimicrobial properties of various forms of sophorolipids)

RN 220608-11-7 HCAPLUS

CN 9-Octadecenoic acid, 17-[(2-0- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

HO
$$\frac{OH}{R}$$
 $\frac{OH}{R}$ $\frac{OH}{$

IT 220608-08-2P 585542-23-0P 585542-25-2P 585542-26-3P 585542-27-4P 585542-28-5P 585542-29-6P 585542-30-9P 585542-31-0P 585542-32-1P 585542-33-2P 585542-34-3P 585542-35-4P 585542-36-5P RL: BPN (Biosynthetic preparation); IMF (Industrial manufacture); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation) (antimicrobial properties of various forms of sophorolipids) RN 220608-08-2 HCAPLUS CN 9-Octadecenoic acid, 17-[[6-O-acetyl-2-O-(6-O-acetyl-β-Dglucopyranosyl)-β-D-glucopyranosyl]oxy]-, butyl ester, (9Z,17S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 585542-23-0 HCAPLUS

CN· 9-Octadecenoic acid, 17-[(6-O-acetyl-2-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-, ethyl ester, (9Z,17S)- (9CI) (CA INDEX NAME)

RN 585542-25-2 HCAPLUS

CN 9-Octadecenoic acid, 17-[[2-O-[6-O-(2-methyl-1-oxo-2-propenyl)- β -D-glucopyranosyl]- β -D-glucopyranosyl]oxy]-, ethyl ester, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 585542-26-3 HCAPLUS

CN 9-Octadecenamide, 17-[(2-O-β-D-glucopyranosyl-β-Dglucopyranosyl)oxy]-N-[2-(4-hydroxyphenyl)ethyl]-, (9Z,17S)- (9CI) (CA
INDEX NAME)

HO S R O Me (CH₂)
$$\frac{1}{6}$$
 $\frac{1}{2}$ (CH₂) $\frac{1}{7}$ OH HO HO HO

RN 585542-27-4 HCAPLUS

CN 9-Octadecenamide, 17-[(2-0- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-N-(2-phenylethyl)-, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 585542-28-5 HCAPLUS

CN 9-Octadecenamide, 17-[(2-O-β-D-glucopyranosyl-β-Dglucopyranosyl)oxy]-N-[2-(4-methylphenyl)ethyl]-, (9Z,17S)- (9CI) (CA
INDEX NAME)

HO S R O Me (CH₂)
$$_{6}$$
 $_{2}$ (CH₂) $_{7}$ O HO HO HO HO

RN 585542-29-6 HCAPLUS
CN 9-Octadecenamide, 17-[(2-O-β-D-glucopyranosyl-β-D-glucopyranosyl) oxy] -N-[2-(4-methoxyphenyl) ethyl]-, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

HO S R O S
$$(CH_2)_6$$
 Z $(CH_2)_7$ O $(CH_2$

RN 585542-30-9 HCAPLUS 9-Octadecenamide, N-[2-(4-fluorophenyl)ethyl]-17-[(2-0- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

HO S R O Me HO OH HO S R O HO S
$$(CH_2)_6$$
 $(CH_2)_7$ O HO HO HO

RN 585542-31-0 HCAPLUS CN 9-Octadecenamide, 17-[[6-0-ace

9-Octadecenamide, 17-[[6-O-acetyl-2-O-(6-O-acetyl- β -D-glucopyranosyl)- β -D-glucopyranosyl]oxy]-N-[2-(4-hydroxyphenyl)ethyl]-, (9Z,17S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 585542-32-1 HCAPLUS

CN 9-Octadecenamide, N-[2-(4-hydroxyphenyl)ethyl]-17-[[6-0-(2-methyl-1-oxo-2-

propenyl) -2-0-[6-0-(2-methyl-1-oxo-2-propenyl) - β -D-glucopyranosyl] - β -D-glucopyranosyl] oxyl -, (9Z,17S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

|| CH₂ PAGE 2-A

RN 585542-33-2 HCAPLUS
CN 9-Octadecenamide, 17-[(6-O-acetyl-2-O-β-D-glucopyranosyl-β-Dglucopyranosyl)oxy]-N-[2-(4-hydroxyphenyl)ethyl]-, (9Z,17S)- (9CI) (CA
INDEX NAME)

RN 585542-34-3 HCAPLUS 9-Octadecenamide, 17-[[2-0- β -D-glucopyranosyl-6-0-(2-methyl-1-oxo-2-propenyl)- β -D-glucopyranosyl]oxy]-N-[2-(4-hydroxyphenyl)ethyl]-, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 585542-35-4 HCAPLUS

9-Octadecenamide, 17-[[2-O-(6-O-acetyl-β-D-glucopyranosyl)-β-D-glucopyranosyl]oxy]-N-[2-(4-hydroxyphenyl)ethyl]-, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 585542-36-5 HCAPLUS 9-Octadecenamide, N-[2-(4-hydroxyphenyl)ethyl]-17-[[2-0-[6-0-(2-methyl-1-oxo-2-propenyl)- β -D-glucopyranosyl]- β -D-glucopyranosyl]oxy]-, (9Z,17S)- (9CI) (CA INDEX NAME)

PAGE 2-A

|| CH₂

IT 220608-05-9P 220608-06-0P 220608-09-3P
RL: BPN (Biosynthetic preparation); IMF (Industrial manufacture); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation) (antimicrobial properties of various forms of sophorolipids)

RN 220608-05-9 HCAPLUS

CN 9-Octadecenoic acid, 17-[[6-O-(1-oxo-2-propenyl)-2-O-[6-O-(1-oxo-2-propenyl)- β -D-glucopyranosyl]- β -D-glucopyranosyl]- β -methyl ester, (9Z,17S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 220608-06-0 HCAPLUS

CN 9-Octadecenoic acid, 17-[[6-O-acetyl-2-O-(6-O-acetyl-β-D-glucopyranosyl)-β-D-glucopyranosyl]oxy]-, methyl ester, (9Z,17S)-(9CI) (CA INDEX NAME)

RN 220608-09-3 HCAPLUS

CN 9-Octadecenoic acid, 17-[[6-O-(3-carboxy-1-oxopropyl)-2-O-[6-O-(3-carboxy-1-oxopropyl)-β-D-glucopyranosyl]-β-D-glucopyranosyl

1-methyl ester, (9Z,17S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

$$HO_2C$$
 OH
 O

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT